Supplement: Iterative Selection Regression (Maller *et al*., 1983)

Procedure fits a lower bound to a data set. The procedure is essentially the same to fit an upper limit line. This Supplement relates to the use of the Excel spreadsheet 'Maller Iterative Selective Regression'.

Step 1

Input **lower points** of the dataset as (xi, yi); Carry out **linear regression** of (xi, yi), shown as in the excel figure; Calculate the **simulated y value** according to the linear regression; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi > y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to "(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2"; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**. In this step, we get the new fitting line "y=0.439542023*x+10.05424883" for use in next step. Besides, the yi which has the highest (yi-y) value should be changed as y in next step.

Step 2

The yi which has the highest (yi-y) in step 1 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 1 "y=0.439542023*x+10.05424883"; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi > y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to "(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2"; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**. In this step, we get the new fitting line "y=0.396965376*x+11.08800981" for use in next step. Besides, the yi which has the highest (yi-y) value should be changed as y in next step.

Step 3

The yi which has the highest (yi-y) in step 2 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 2 “y=0.396965376*x+11.08800981”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi＞y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**. In this step, we get the new fitting line “y=0.361582237*x+18.29484759” for use in next step. Besides, the yi which has the highest (yi-y) value should be changed as y in next step.

Step 4

The yi which has the highest (yi-y) in step 3 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 3 “y=0.361582237*x+18.29484759”; Calculate **the difference between yi and y**; As all yi<y, Carry out **linear regression** of (xi, yi), shown as the figure. In this step, we get the new fitting line “y=0.3606*x+8.8597” for use in next step.

Step 5

Calculate **simulated y value** according to linear regression in step 4 “y=0.3606*x+8.8597”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi＞y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**.

In this step, we get the new fitting line “y=0.335008828*x+14.07210984” for use in next step. Besides, the yi which has the highest (yi-y) value should be changed as y in next step.

Step 6

The yi which has the highest (yi-y) in step 5 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 5 “y=0.335008828*x+14.07210984”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi＞y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**. In this step, we get the new fitting line “y= 0.317109702*x+15.25577904” for use in next step. Besides, the yi which has the highest (yi-y) should be changed as y in next step.

Step 7

The yi which has the highest (yi-y) in step 6 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 6 “y= 0.317109702*x+15.25577904”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi＞y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**. In this step, we get the new fitting line “y=0.305387181*x+17.64342214” for use in next step. Besides, the yi which has the highest (yi-y) should be changed as y in next step.

Step 8

The yi which has the highest (yi-y) in step 7 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 7 “y=0.305387181*x+17.64342214”; Calculate **the difference between yi and y**; As all yi<y, Carry out **linear regression** of (xi, yi), shown as in the figure. In this step, we get the new fitting line “y=0.3054*x+12.352” for use in next step.

Step 9

Calculate **simulated y value** according to linear regression in step 8 “y=0.3054*x+12.352”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi＞y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**.

In this step, we get the new fitting line “y=0.289271609*x+15.6372306” for use in next step. Besides, the yi which has the highest (yi-y) should be changed as y in next step.

Step 10

The yi which has the highest (yi-y) in step 9 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 9 “y=0.289271609*x+15.6372306”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi＞y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**. In this step, we get the new fitting line “y=0.282076325*xi+16.11305474” for use in next step. Besides, the yi which has the highest (yi-y) should be changed as y in next step.

Step 11

The yi which has the highest (yi-y) in step 10 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 10 “y=0.282076325*xi+16.11305474”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi＞y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**.

In this step, we get the new fitting line “y=0.361582237*x+18.29484759” for use in next step. Besides, the yi which has the highest (yi-y) value should be changed as y in next step.

Step 12

The yi which has the highest (yi-y) in step 11 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step 11 “y=0.361582237*x+18.29484759”; Calculate **the difference between yi and y**; Calculate the **average value of xi**; Calculate the **difference between xi and xave**; Calculate the **sum of (xi-xave)^2** ; When **yi<y, calculate yi*(xi-xave)** and the sum value, when **yi > y, calculate y*(xi-xave)** and the sum value; Calculate the **slope of new fitting line** according to “(sum of yi*(xi-xave)+ sum of y*(xi-xave))/ sum of (xi-xave)^2”; According to the point which has the highest (yi-y), calculate the **intercept of the new fitting line**.

In this step, we get the new fitting line “y=0.361582237*x+18.29484759” for use in next step. Besides, the yi which has the highest (yi-y) value should be changed as y in next step.

Step 13

The yi which has the highest (yi-y) in step 12 should be changed as y; Calculate the **simulated y value** according to the calculated fitting line in step12 “y=0.361582237*x+18.29484759”; Calculate **the difference between yi and y**; As all yi<y, Carry out **linear regression** of (xi, yi), shown as the figure. In this step, we get the new fitting line “y=0.2774x+13.998”.

As R^2=0.9577>0.95, we get the final lower boundary “y=0.2774x+13.998”.